REPORT DOCUMENTATION PAGE

Form Approved OMB NO. 0704-0188

1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
13-01-2015	Final Report	12-Jan-2010 - 30-Sep-2014

4. TITLE AND SUBTITLE	
Final Report: Nanoengineered Carbon-Based Materials For Reactive Adsorption of Toxic Industrial Compounds	5a. CONTRACT NUMBER W911NF-10-1-0030
	5b. GRANT NUMBER
	5c. PROGRAM ELEMENT NUMBER 622622
6. AUTHORS Teresa J. Bandosz	5d. PROJECT NUMBER
	5e. TASK NUMBER
	5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAMES AND ADDRESSES	8. PERFORMING ORGANIZATION REPORT NUMBER
CUNY - City College of New York Research Foundation of CUNY 230 W 41st Street FL 7 New York, NY 10036 -7207	

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS (ES)	10. SPONSOR/MONITOR'S ACRONYM(S) ARO
U.S. Army Research Office P.O. Box 12211 Research Triangle Park, NC 27709-2211	11. SPONSOR/MONITOR'S REPORT NUMBER(S) 57373-CH-H.68

12. DISTRIBUTION AVAILIBILITY STATEMENT

Approved for Public Release; Distribution Unlimited

13. SUPPLEMENTARY NOTES

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14. ABSTRACT

Composites of Cu-BTC and hydroxides of zinc, zirconium, copper and cobalt were synthesized. They were characterized from the view points of their porosity and surface and used as adsorbents of H2S, NH3, NO2, CO2. The results showed that the addition of carbonaceous phase increased the surface area and significantly affected the chemistry of the composites. The resulting hydroxide composites were very amorphous with developed surface area and the high content of terminal hydroxyl groups important for reactive adsorption of toxic gases. When the

15. SUBJECT TERMS

Toxic industrial compounds, composite adsorbents, reactive adsorption, surface chemistry, toxic gases removal

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Teresa Bandosz
UU	UU	UU	UU		19b. TELEPHONE NUMBER 212-650-6017

Standard Form 298 (Rev 8/98)
Prescribed by ANSI Std. Z39.18

Report Title

Final Report: Nanoengineered Carbon-Based Materials For Reactive Adsorption of Toxic Industrial Compounds

ABSTRACT

Composites of Cu-BTC and hydroxides of zinc, zirconium, copper and cobalt were synthesized. They were characterized from the view points of their porosity and surface and used as adsorbents of H2S, NH3, NO2, CO2. The results showed that the addition of carbonaceous phase increased the surface area and significantly affected the chemistry of the composites. The resulting hydroxide composites were very amorphous with developed surface area and the high content of terminal hydroxyl groups important for reactive adsorption of toxic gases. When the hydroxide of semiconductive properties was used, the samples exhibited photoactivity enhanced by the presence of graphene phase. That phase contributed to the separation of photoinduced charges and prevented their recombination leading to more efficient redox reaction. In the case of MOF /GO composites addition of GO increased in the degree of surface heterogeneity and thus formed more reactive centers for adsorption. When zirconium based MOF were modified (with an amine or Ce) the adsorption capacity for NO2 significantly increased. While in the case of H2S, water increased the amount adsorbed, a mixed effect was found for NO2 adsorption. On the materials obtained very high adsorption capacities for the removal of toxic gases and CO2 were measured.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received		Paper
01/03/2011	8.00	S. Bashkova, D. Deoki, T J. Bandosz. Effect of silver nanoparticles deposited on micro/mesoporous activated carbons on retention of NOx at room temperature, Journal of Colloid and Interface Science, (10 2010): . doi:
01/03/2011	10.00	C. Petit, B. Mendoza, T.J Bandosz. Hydrogen Sulfide Adsorption on Metal-Organic Frameworks and Metal-Organic Frameworks / Graphite Oxide Composites, ChemPhysChem, (11 2010): . doi:
01/03/2011	9.00	Benoit Levasseur, Camille Petit, Teresa J. Bandosz. Reactive adsorption of NO2 on copper-based MOF and Graphite oxide-MOF composites, ACS Applied Materials and Interfaces, (11 2010): . doi:
01/03/2011	1.00	M. Seredych, T.J. Bandosz. Effects of surface features on adsorption of SO2 on graphite oxide/Zr(OH)4 composites , Journal of Physical Chemistry C, (07 2010): . doi:
01/03/2011	7.00	C. Petit, J. Burress, T.J. Bandosz. The synthesis and characterization of copper-based metal organic framework/graphene composites, Carbon, (9 2010): . doi:
01/03/2011	6.00	C. Petit, B. Mendoza, T.J. Bandosz. Reactive adsorption of ammonia on Cu-based MOF /graphene composites , Langmuir, (7 2010): . doi:
01/13/2015	62.00	Kavindra Singh, Nikolina A. Travlou, Svetlana Bashkova, Enrique Rodríguez-Castellón, Teresa J. Bandosz. Nanoporous carbons as gas sensors: Exploring the surface sensitivity, Carbon, (12 2014): 0. doi: 10.1016/j.carbon.2014.08.055
01/13/2015	57.00	Alfonso Policicchio, Yunxia Zhao, Qin Zhong, Raffaele G. Agostino, Teresa J. Bandosz. Cu-BTC/Aminated Graphite Oxide Composites As High-Efficiency CO, ACS Applied Materials & Interfaces, (01 2014): 0. doi: 10.1021/am404952z
01/13/2015	60.00	Liangliang Huang, Mykola Seredych, Teresa J. Bandosz, Adri C. T. van Duin, Xiaohua Lu, Keith E. Gubbins. Controllable atomistic graphene oxide model and its application in hydrogen sulfide removal, The Journal of Chemical Physics, (11 2013): 0. doi: 10.1063/1.4832039
01/13/2015	65.00	Amani Ebrahim, Teresa J. Bandosz. Ce(III) Doped Zr-Based MOFs as Excellent NO2 Adsorbents atAmbient Conditions, ACS Applied Materials and Interfaces, (10 2013): 10565. doi:
01/13/2015	67.00	Amani M. Ebrahim, Benoit Levasseur, Teresa J. Bandosz. Interactions of NO2 with Zr-Based MOF: Effects of the Size of OrganicLinkers on NO2 Adsorption at Ambient Conditions, ACS Applied Materials and Interfaces, (12 2012): 168. doi:
01/13/2015	59.00	Yunxia Zhao, Mykola Seredych, Jacek Jagiello, Qin Zhong, Teresa J. Bandosz. Insight into the mechanism of CO2 adsorption on Cu–BTC and its composites with graphite oxide or aminated graphite oxide, Chemical Engineering Journal, (03 2014): 0. doi: 10.1016/j.cej.2013.11.037

01/13/2015 63.00 Marc Florent, Teresa J. Bandosz. Effects of surface heterogeneity of cobalt oxyhydroxide/graphite oxide composites on reactive adsorption of hydrogen sulfide,
Microporous and Mesoporous Materials, (03 2015): 0. doi: 10.1016/j.micromeso.2014.11.001

01/13/2015 66.00 Svetlana Bashkova, Teresa J. Bandosz. Insight into the role of the oxidized graphite precursor on the propertiesof copper-based MOF/graphite oxide composites,
Microporous and Mesoporous Materials, (11 2013): 205. doi:

01/13/2015 58.00 Svetlana Bashkova, Teresa J. Bandosz. Effect of surface chemical and structural heterogeneity of copper-based MOF/graphite oxide composites on the adsorption of ammonia,
Journal of Colloid and Interface Science, (03 2014): 0. doi: 10.1016/j.jcis.2013.11.010

01/13/2015 61.00 Dimitrios A. Giannakoudakis, Teresa J. Bandosz. Zinc (hydr)oxide/graphite oxide/AuNPs composites: Role of surface features in H2S reactive adsorption,
Journal of Colloid and Interface Science, (12 2014): 0. doi: 10.1016/j.jcis.2014.08.046

01/13/2015 64.00 Camille Petit, Teresa J. Bandosz. Engineering the surface of a new class of adsorbents: Metal–organic framework/graphite oxide composites,
Journal of Colloid and Interface Science, (08 2014): 0. doi: 10.1016/j.jcis.2014.08.026

08/06/2013 52.00 Yohann Corre, Mykola Seredych, Teresa J. Bandosz. Analysis of the chemical and physical factors affecting reactive adsorption of ammonia on graphene/nanoporous carbon composites,
Carbon, (4 2013): 0. doi: 10.1016/j.carbon.2012.12.024

08/06/2013 54.00 Oluwaniyi Mabayoje, Mykola Seredych, Teresa J. Bandosz. Reactive adsorption of hydrogen sulfide on visible light photoactive zinc (hydr)oxide/graphite oxide and zinc (hydr)oxychloride/graphite oxide composites,
Applied Catalysis B: Environmental, (3 2013): 0. doi: 10.1016/j.apcatb.2012.12.011

08/06/2013 44.00 Yunxia Zhao, Mykola Seredych, Qin Zhong, Teresa J. Bandosz. Aminated graphite oxides and their composites with copper-based metal–organic framework: in search for efficient media for CO2 sequestration,
RSC Advances, (03 2013): 0. doi: 10.1039/c3ra40817e

08/06/2013 48.00 Yunxia Zhao, Mykola Seredych, Qin Zhong, Teresa J. Bandosz. Superior Performance of Copper Based MOF and Aminated Graphite Oxide Composites as CO,
ACS Applied Materials & Interfaces, (06 2013): 0. doi: 10.1021/am4006989

08/06/2013 46.00 Liangliang Huang, Teresa Bandosz, Kaushik L. Joshi, Adri C. T. van Duin, Keith E. Gubbins. Reactive adsorption of ammonia and ammonia?water on CuBTC metal-organic framework: A ReaxFF molecular dynamics simulation,
The Journal of Chemical Physics, (2013): 0. doi: 10.1063/1.4774332

08/06/2013 51.00 Mykola Seredych, Oluwaniyi Mabayoje, Teresa J. Bandosz. Involvement of water and visible light in the enhancement in SO2 adsorption at ambient conditions on the surface of zinc (hydr)oxide/graphite oxide composites,
Chemical Engineering Journal, (5 2013): 0. doi: 10.1016/j.cej.2013.03.026

08/06/2013 45.00 Teresa J. Bandosz, Robert Alfano, SM. Z. Islam, Taposh Gayen, Bidyut B. Das, Lingyan Shi, Mykola Seredych, Alaa Moussawi. Time-resolved photoluminescence of Zn(OH)_2 and its composites with graphite oxides,
Optics Letters, (06 2013): 0. doi: 10.1364/OL.38.002227

08/06/2013 50.00 SM Z. Islam, Taposh Gayen, Alaa Moussawi, Lingyan Shi, Mykola Seredych, Teresa J. Bandosz, Robert Alfano. Structural and optical characterization of Zn(OH)_2and its composites with graphite oxides,
Optics Letters, (03 2013): 0. doi: 10.1364/OL.38.000962

08/06/2013 49.00 Amani M. Ebrahim, Benoit Levasseur, Teresa J. Bandosz. Effects of Carbon Phase Deposition in Silica Gel Pores on NO,
Langmuir, (06 2013): 0. doi: 10.1021/la4008137

08/06/2013 53.00 Amani M. Ebrahim, Benoit Levasseur, Teresa J. Bandosz. Interactions of NO,
Langmuir, (01 2013): 0. doi: 10.1021/la302869m

08/06/2013 42.00 Oluwaniyi Mabayoje, Mykola Seredych, Teresa J. Bandosz. Enhanced adsorption of hydrogen sulfide on mixed zinc/cobalt hydroxides: Effect of morphology and an increased number of surface hydroxyl groups, Journal of Colloid and Interface Science, (9 2013): 0. doi: 10.1016/j.jcis.2013.05.006

08/06/2013 47.00 Marc Florent, Marialaura Tocci, Teresa J. Bandosz. NO2 adsorption at ambient temperature on urea-modified ordered mesoporous carbon, Carbon, (07 2013): 0. doi: 10.1016/j.carbon.2013.06.081

08/09/2011 15.00 Camille Petit, Karifala Kante, Teresa J. Bandosz. The role of sulfur-containing groups in ammonia retention on activated carbons, Carbon, (03 2010): 0. doi: 10.1016/j.carbon.2009.10.007

08/09/2011 17.00 Benoit Levasseur, Camille Petit, Teresa J. Bandosz. Reactive Adsorption of NO, ACS Applied Materials & Interfaces, (12 2010): 0. doi: 10.1021/am100790v

08/09/2011 23.00 Barbara Mendoza, Camille Petit, Teresa J. Bandosz. Hydrogen Sulfide Adsorption on MOFs and MOF/Graphite Oxide Composites, ChemPhysChem, (12 2010): 0. doi: 10.1002/cphc.201000689

08/09/2011 26.00 Camille Petit, Teresa J. Bandosz. MOF / Graphite oxide hybrid materials: Exploring the New Concept of Adsorbents and Catalysts, Adsorption, (01 2011): 5. doi:

08/09/2011 14.00 Mykola Seredych, Teresa J. Bandosz. Reactive adsorption of hydrogen sulfide on graphite oxide/Zr(OH)4 composites, Chemical Engineering Journal, (02 2011): 0. doi: 10.1016/j.cej.2010.11.096

08/09/2011 19.00 Eleni Deliyanni, Teresa J. Bandosz. Effect of Carbon Surface Modification with Dimethylamine on Reactive Adsorption of NO, Langmuir, (03 2011): 0. doi: 10.1021/la1042537

08/09/2011 20.00 Benoit Levasseur, Eugene Gonzalez-Lopez, Joseph A. Rossin, Teresa J. Bandosz. Effect of Reduction Treatment on Copper Modified Activated Carbons on NO, Langmuir, (05 2011): 0. doi: 10.1021/la104948d

08/09/2011 13.00 Svetlana Bashkova, Deeona Deoki, Teresa J. Bandosz. Effect of silver nanoparticles deposited on micro/mesoporous activated carbons on retention of NOx at room temperature, Journal of Colloid and Interface Science, (02 2011): 0. doi: 10.1016/j.jcis.2010.10.031

08/09/2011 11.00 Mykola Seredych, Joseph A. Rossin, Teresa J. Bandosz. Changes in graphite oxide texture and chemistry upon oxidation and reduction and their effect on adsorption of ammonia, Carbon, (11 2011): 0. doi: 10.1016/j.carbon.2011.06.032

08/14/2012 34.00 Mykola Seredych, Teresa J. Bandosz, Oluwaniyi Mabayoje. Cobalt (hydr)oxide/graphite oxide composites: Importance of surface chemical heterogeneity for reactive adsorption of hydrogen sulfide, Journal of Colloid and Interface Science, (7 2012): 0. doi: 10.1016/j.jcis.2012.04.007

08/14/2012 28.00 Mykola Seredych, Teresa J. Bandosz, Oluwaniyi Mabayoje. Enhanced Reactive Adsorption of Hydrogen Sulfide on the Composites of Graphene/Graphite Oxide with Copper (Hydr)oxychlorides, ACS Applied Materials & Interfaces, (06 2012): 0. doi: 10.1021/am300702a

08/14/2012 27.00 Teresa J. Bandosz, Matt Laskoski, John Mahle, Gregory Mogilevsky, Gregory W. Peterson, Joseph A. Rossin, George W. Wagner. Reactions of VX, GD, and HD with Zr(OH), The Journal of Physical Chemistry C, (05 2012): 0. doi: 10.1021/jp3028879

08/14/2012 30.00 Mykola Seredych, Oluwaniyi Mabayoje, Teresa J. Bandosz. nteractions of NO2 with Zinc (Hydr) oxide/Graphene Phase Composites: Visible Light Enhanced Surface Reactivity, The Journal of Physical Chemistry C, (01 2012): 0. doi: 10.1021/jp211141j

08/14/2012 37.00 Karifala Kante, Cesar Nieto-Delgado, J. Rene Rangel-Mendez, Teresa J. Bandosz. Spent coffee-based activated carbon: Specific surface features and their importance for H2S separation process, Journal of Hazardous Materials, (1 2012): 0. doi: 10.1016/j.jhazmat.2011.11.053

08/14/2012 39.00 Benoit Levasseur, Amani M. Ebrahim, Jacob Burress, Teresa J. Bandosz. Interactions of NO2 at ambient temperature with cerium–zirconium mixed oxides supported on SBA-15,
Journal of Hazardous Materials, (12 2011): 0. doi: 10.1016/j.jhazmat.2011.09.087

08/14/2012 41.00 Camille Petit, Teresa J. Bandosz. Explorination chemistry of MOF–graphite oxide composites and their applications as adsorbents,
Dalton Transactions, (2012): 0. doi: 10.1039/c2dt12017h

08/14/2012 35.00 Teresa J. Bandosz. Towards understanding reactive adsorption of small molecule toxic gases on carbonaceous materials,
Catalysis Today, (6 2012): 0. doi: 10.1016/j.cattod.2011.08.017

08/14/2012 36.00 Camille Petit, Benoit Levasseur, Barbara Mendoza, Teresa J. Bandosz. Reactive adsorption of acidic gases on MOF/graphite oxide composites,
Microporous and Mesoporous Materials, (5 2012): 0. doi: 10.1016/j.micromeso.2011.09.012

08/14/2012 38.00 Mykola Seredych, Teresa J. Bandosz. Manganese oxide and graphite oxide/MnO2 composites as reactive adsorbents of ammonia at ambient conditions,
Microporous and Mesoporous Materials, (3 2012): 0. doi: 10.1016/j.micromeso.2011.09.010

08/14/2012 33.00 Benoit Levasseur, Amani M. Ebrahim, Teresa J. Bandosz. Mesoporous silica SBA-15 modified with copper as an efficient NO2 adsorbent at ambient conditions,
Journal of Colloid and Interface Science, (7 2012): 0. doi: 10.1016/j.jcis.2012.03.072

08/14/2012 40.00 Mykola Seredych, Oluwaniyi Mabayoje, Maria M. Kole?nik, Vojislav Krsti?, Teresa J. Bandosz. Zinc (hydr) oxide/graphite based-phase composites: effect of the carbonaceous phase on surface properties and enhancement in electrical conductivity,
Journal of Materials Chemistry, (2012): 0. doi: 10.1039/c2jm15350e

08/14/2012 32.00 Liangliang Huang, Jacek Jagiello, Camille Petit, Jeffrey Kenvin, Keith E. Gubbins, Teresa J. Bandosz. Toward Understanding Reactive Adsorption of Ammonia on Cu-MOF/Graphite Oxide Nanocomposites,
Langmuir, (11 2011): 0. doi: 10.1021/la202924y

08/14/2012 31.00 Benoit Levasseur, Amani M. Ebrahim, Teresa J. Bandosz. Interactions of NO2 with Amine-Functionalized SBA-15: Effects of Synthesis Route,
Langmuir, (04 2012): 0. doi: 10.1021/la300371m

08/14/2012 29.00 Teresa J. Bandosz, Mykola Seredych, Oluwaniyi Mabayoje. Visible-Light-Enhanced Interactions of Hydrogen Sulfide with Composites of Zinc (Oxy)hydroxide with Graphite Oxide and Graphene,
Langmuir, (01 2012): 0. doi: 10.1021/la204277c

09/27/2013 56.00 Svetlana Bashkova, Teresa J. Bandosz. Insight into the role of the oxidized graphite precursor on the properties of copper-based MOF/graphite oxide composites,
Microporous and Mesoporous Materials, (09 2013): 0. doi: 10.1016/j.micromeso.2013.06.002

TOTAL: **54**

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received	Paper
08/09/2011 12.00	Jacob Burress, Camille Petit, Teresa J. Bandosz. The synthesis and characterization of copper-based metal–organic framework/graphite oxide composites, Carbon, (02 2011): 0. doi: 10.1016/j.carbon.2010.09.059
08/09/2011 16.00	Mykola Seredych, Teresa J. Bandosz. Effects of Surface Features on Adsorption of SO, The Journal of Physical Chemistry C, (08 2010): 0. doi: 10.1021/jp1051479
08/09/2011 18.00	Camille Petit, Barbara Mendoza, Teresa J. Bandosz. Reactive Adsorption of Ammonia on Cu-Based MOF/Graphene Composites, Langmuir, (10 2010): 0. doi: 10.1021/la1021092
08/09/2011 21.00	Benoit Levasseur, Amani M. Ebrahim, Teresa J. Bandosz. Role of Zr, Langmuir, (07 2011): 0. doi: 10.1021/la201338w
08/09/2011 22.00	Camille Petit, Barbara Mendoza, Deanna O'Donnell, Teresa J. Bandosz. Effect of Graphite Features on the Properties of Metal–Organic Framework/Graphite Hybrid Materials Prepared Using an in Situ Process, Langmuir, (08 2011): 0. doi: 10.1021/la2017424
08/09/2011 24.00	Svetlana Bashkova, Teresa J. Bandosz. Reactive Adsorption of NO2 at Ambient Conditions on Iron-Containing Polymer-Based Porous Carbons, ChemSusChem, (03 2011): 0. doi: 10.1002/cssc.201000296
08/09/2011 25.00	Camille Petit, Teresa J. Bandosz. Synthesis, Characterization, and Ammonia Adsorption Properties of Mesoporous Metal-Organic Framework (MIL(Fe))-Graphite Oxide Composites: Exploring the Limits of Materials Fabrication, Advanced Functional Materials, (06 2011): 0. doi: 10.1002/adfm.201002517

TOTAL: **7**

Number of Papers published in non peer-reviewed journals:

(c) Presentations

1 1. Effects of structural and Chemical heterogeneity of zinc hydroxide/graphite oxide/AuNP on the Reactive adsorption of Hydrogen sulfide
D. Giannkoudakis, T.J. Bandosz
4th World Colloid Conference: Surface design and Engineering. Madrid Spain, June 15-18, 2014;
2. MOF/GO composites: Exploring the concept of new separation media
Teresa J. Bandosz
4th World Colloid Conference: Surface design and Engineering. Madrid Spain, June 15-18, 2014; Plenary lecture

3. Superior performance of MOF/aminated oxide composites as adsorbents of CO_2.
Y. Zhao, M. Seredych and T.J. Bandosz
PPM 2013, September 3-7, Cesme, Turkey.

4. Superior performance of MOF/aminated oxide composites as adsorbents of CO_2.
Y. Zhao, M. Seredych and T.J. Bandosz
XXII ICCDU, June 23-25, 2013 Alexandria, Viginia,

5. Reactive Adsorption of Sulfur containing gases on $Zn(OH)_2$ graphite oxide composites .
Mykola Seredych, Oluwaniyi Mabayoje, and Teresa J. Bandosz. Hybrid Materials 2013, Sorrento, Italy, March 3-7, 2013.

6. Towards understanding reactive adsorption of toxic gases on carbonaceous adsorbents. Plenary lecture.
Teresa J. Bandosz
2-nd South American Conference of Adsorbents and Adsorption. San Luis, Argentina, February 20-23, 2013.

7. Towards understanding reactive adsorption of toxic gases on carbonaceous adsorbents. Invited lecture.
T. J. Bandosz.
Federal University of Ceara, Fortaleza, Brazil, January 23, 2013.

8. Visible-Light-Enhanced Interactions of Hydrogen Sulfide with Composites of Zinc (Oxy)hydroxide with Graphite Oxide and Graphene
M. Seredych, O. Mabayoje, T. J. Bandosz
ISSHAC-8, August 29-Sept. 3, 2012.

9. Visible-Light-Enhanced Interactions of Hydrogen Sulfide with Composites of Zinc (Oxy)hydroxide with Graphite Oxide and Graphene
M. Seredych, O. Mabayoje, T. J. Bandosz
IBA-1, Recife, Brazil, May 5-May 10, 2012.

10. Graphite oxide/ $Zn(OH)_2$ composites as adorbents of sulfur containing gases
CPP-6, Delray Beach, Florida March 29-April 2 , 2012
M. Seredych, O. Mabayoje, T. J. Bandosz

11. Visible-Light-Enhanced Interactions of Hydrogen Sulfide with Composites of Zinc (Oxy)hydroxide with Graphite Oxide and Graphene.
M. Seredych, O. Mabayoje, T. J. Bandosz
Applications of Carbons in Energy, Am.C.S. Workshop, Atlanta, GO, March 29-30, 2012

12. MOF/Graphene composites: Exploring the limits of materials preparation
C.Petit, Benoit Levasseur, Barbara Mendoza and T.J. Bandosz
Carbon 2011, July 23-28, Shanghai, China.

13. Adsorption of acidic gases on MOF/Graphite oxide composites
C.Petit, Benoit Levasseur, Barbara Mendoza and T.J. Bandosz
COPS-IX, Dresden Germany, June 5-8, 2011.

14. MOF-Graphene composites: Exploring the new concept of adsorbents and Catalysts for removal of toxic gases
C.Petit, T.J. Bandosz
Decon 2010 Conference, Lake Louis, Canada, September 28-30, 2010.

15. MOF/Graphene composites: exploring a new concept of adsorbents and catalysts
C. Petit, T.J. Bandosz
Abstracts Brazilian Meeting of Chemical Engineers and Brazilian Adsorption Society, Iguassu Fall, Brazil, September 19-22, 2010

16. MOF/Graphene composites: exploring a new concept of adsorbents
C. Petit and T.J. Bandosz

Extended Abstracts of Carbon 2010, Clemson, SC, July 11-16, 2010

17. MOF/Graphene composites as adsorbents of toxic gases
C. Petit and T.J. Bandosz
Abstracts of FOA-9, Awaji Island, Japan, May 22-25, 2010

Number of Presentations: 17.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received		Paper
01/03/2011	2.00	C. Petit, T . J. Bandosz. MOF / Graphite oxide hybrid materials: Exploring the New Concept of Adsorbents and Catalysts, (08 2010)
01/03/2011	3.00	S. Bashkova, T.J. Bandosz. Adsorption of NO2 at room temperature on iron-containing polymer-based porous carbons, ChemSusChem (01 2011)
01/03/2011	4.00	M. Seredych, T.J. Bandosz. Reactive Adsorption of Hydrogen Sulfide on Graphite oxide/Zr(OH)4 composites, (11 2010)
01/03/2011	5.00	Eleni Deliyanni, Teresa J. Bandosz. Effect of Carbon Surface Modification with Dimethylamine on Reactive Adsorption of NOx, Langmuir (12 2010)

TOTAL: **4**

Number of Manuscripts:

Books

Received Book

TOTAL:

Received Book Chapter

TOTAL:

Patents Submitted

Patents Awarded

Compositions comprising zirconium hydroxide
and graphite oxide and methods for use
US 8658555 B1
Teresa J. Bandosz, Mykola Seredych,
Gregory W. Peterson, Christopher J. Karwacki

Awards

The PI became the editor of the Journal of Colloid and Interface Science (Elsevier)

Graduate Students

NAME	PERCENT_SUPPORTED	Discipline
Yunxia Zhao	0.00	
NIkolina Travlou	0.50	
Dimitrios GIannakoudakis	0.50	
FTE Equivalent:	**1.00**	
Total Number:	**3**	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
Svetlana Bashova	0.30
Benoit Levassur	1.00
Marc Florent	1.00
Mykola Seredych	0.00
FTE Equivalent:	**2.30**
Total Number:	**4**

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Teresa J. Bandosz	0.10	
FTE Equivalent:	**0.10**	
Total Number:	**1**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED	Discipline
Oluwaniy Mabayoye	0.20	Chemistry
Kavindra Singh	0.10	Chemical Engineering
Rajiv Wallace	0.10	Chemical Engineering
Jacon Marcus	0.20	Chemistry
FTE Equivalent:	**0.60**	
Total Number:	**4**	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 2.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:...... 2.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:...... 1.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):...... 2.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:...... 1.00

Names of Personnel receiving masters degrees

NAME	
Amani Ebrahim	
Total Number:	**1**

Names of personnel receiving PHDs

NAME

Total Number:

Names of other research staff

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

Key achievements

1. Zn(OH)2/Graphite oxide and Zn(OH)2/Graphene composites are very promising materials exhibiting high H2S, SO2 as well as NO2 adsorption capacities.
2. Zn(OH)2 /graphene phase composites show very interesting photoactivity in visible light. It enhances the reactive adsorption process
3. Grafting of amines on the surface of SBA-15 creates good adsorbents for both NO2 and NO. Unfortunately, they are active only in dry conditions.
4. UIP-66 and its composites with graphite oxide show promising properties for adsorption of NO2 both in dry and wet conditions
5. Co(OH)2/Graphite oxide and Co(OH)2/Graphene composites are promising materials exhibiting high H2S, adsorption capacities.
6. Hydrophobization of silica surface followed by deposition of mixed zicronia/ceria oxides results in insensitivity of the adsorbent to water. Moisture in air does not decreases the performance as NO2 adsorbents.
7. Cu(OH)2/Graphite oxide and Co(OH)2/Graphene composites are promising materials exhibiting high H2S, adsorption capacities.
8. Addition of 10 % calex(4)arenes to mesoporous carbon decreased the surface significantly. In spite of this decrease the NO2 adsorption became unchanged and the NO emission decreased.
9. Photoactivity of composites with GO has a potential to open new research path to increase the efficiency of reactive adsorption at ambient conditions
10. The new urea-modified graphite oxide-HUST-1 exhibit very unique textural and chemical features. The synergistic effects of composite formation are clearly demonstrated. They are linked the defects in the MOF structure
11. The properties of the composites are governed by the properties of GO used to build the composites
12. The cobalt/zinc mixed hydroxides/ GO with heterogeneous amorphous structures were synthesized. The synergistic effects of the composite formation on the surface features were identified.
13. The photoacivity of cobalt/zinc mixed hydroxides/ GO in visible light (an increase in the amount of H2S adsorbed) was linked to oxidation of cobalt, oxygen defects and the increased conductivity due to the presence of graphene phase.
14. Mesoporous carbon and its nitrogen nitrogen-modified counterparts are good NO2 adsorbents.
15. Mesoporous silica/carbon composites exhibit good NO2 adsorption capacity in the presence of water owing to carbons hydrophobicity and a decrease in the extent of competition for adsorption centers between water and NO2
16. Very high adsorption capacities either at ambient or high pressure for CO2 were measured on new MOF/GO-U and MOF/GO composites.
17. The MOF/GO composites show good performance in the presence of methane. This means that reactive adsorption is predominant and methane is not adsorbed or if it is, it does not interfere with the surface reactive centers.
18. Synthesis of UiO-66 and UIO-67 in the presence of cerium resulted in a new hybrid MOF.
19. The amount of NO2 adsorbed on the Ce-doped MOF increases over 25% in dry conditions in comparison with the unmodified MOF. Exposure of Ce-UiO-66 to NO2 results in a development of porosity. Regardless the conditions, the XRD patterns indicate the stability of this new hybrid MOF upon NO2 adsorption. Interactions of NO2 with MOF result in the formation of nitrate and nitrite species
20. On the Ce-UiO-66 and Ce-UiO-67 an improvement in the NO2 adsorption capacity is found in both, dry and wet, conditions in comparison with those on the parent MOFs.
21. Ordered mesporous carbons modified with nitrogen are shown as good NO2 adsorbents in both dry and wet conditions. This is owing to the favorable distribution of specific nitrogen groups existing in larger pores were adsorption can take place.
22. A high degree of surface amorphicity accompanied by a high number of OH groups on the surface of mixed Zn/Co hydroxide were found as crucial factors factor determining their good performance as reactive adsorbents of hydrogen sulfide.
23. Introducing Lewis basic sites to zirconium carboxylic acid based materials by the incorporation of –NH2 groups promotes chemical reactions on the surface. The amine (NH2) or the carbonyl (C=O) groups in urea directly interact with NO2 molecules in both moist and dry conditions, which leads to the formation of surface bound nitrates.
24. In the case of melamine modified zirconium carboxylic acid based materials the hydrolysis of the terminal secondary –NH2 creates oxygen rich functional groups that cause the formation of surface bound nitrate species.
25. CoOOH is a good adsorbent of hydrogen sulfide. Adsorption in moist condition is about twice more effective than in dry conditions. In all cases, the desorption is sharp implying that H2S is strongly bonded to the surface. Very little SO2 was detected during the adsorption in dry conditions. A release of 0.0024 %, 0.0016 % and 0.0008 % was measured for CoOOH, CoOOH-GO1 and CoOOH-GO10 respectively. This seems to indicate that GO may react with SO2, limiting its release.
26. All Cd/GO materials are good adsorbents in moist conditions toward H2S, Cd(OH)2-based materials are better adsorbents than CdCO3-based ones. Adding 1% GO decreases the capacity of the materials. On the other hand, adding 10% GO restores that capacity, giving a slightly higher capacity in the case of CdCO3 and a slightly lower capacity in the case of Cd(OH)2
27. The HKUST-1 sulfur doped GO are excellent adsorbents of hydrogen sulfide. Up to 144 and 240 mg/g in dry and moist conditions, respectively, are adsorbed on the surface.
28. We have usefully developed an environmentally friendly route for the incorporation of N, and S functionalities via solvothermal methods. The nature of the modifier results in different chemical features and distinct morphologies. The surface of the modified GO samples is abundant in phenolic, sulfonic, thioethers and pyrrolic groups.
29. Addition of small amount of sulfanilic acid (grafting with acid) to silica-carbons composites increases NO2 adsorption which

might be via polar interactions and specific interactions with amines.

30. The composites with iron oxide with different levels of iron oxidation significantly differ in their performance as hydrogen sulfide adsorbents
31. The oxidation level of iron seem to be more important than the developed surface area
32. Addition of GO to magnetite increases the capacity for H_2S removal more than 3 times. That increase is linked to an increase in hydrophilicity level, in surface area and to a decrease in the average size of pores.
33. The behavior of MOF/S-doped graphite oxides adsorbed of TIC differ depending on the kind of S-doped GO used for synthesis.
34. The ZnOH/GO/AuNPs composite exhibited the greatest H_2S adsorption capacity due to the increased number of OH terminal groups and the conductive properties of GO that facilitated the electron transfer and consequently the formation of superoxide ions promoting oxidation of hydrogen sulfide. AuNPs present in the composite increased the conductivity, helped with electron transfer to oxygen, and prevented the fast recombination of the electrons and the holes.
35. The new application of nanoporous carbon as toxic gas sensors was proposed and explored. The materials show very promising properties linking the detection and protection functions.
36. The MOF/GO composites were tested for the firs time as toxic gas sensors. Changes in conductivity are measurable and they depend on the chemistry of the composites

Technology Transfer

Key achievements

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